P.I.: Tuncay Aktosun

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FINAL PROJECT REPORT

The material profile of a thin film can be analyzed by placing the film on a substrate and by sending a neutron beam onto it at various angles of incidence. Technically, the scattering length density of the film needs to be determined as a function of depth. A reflectometer is used to measure the amount of reflection (reflectivity) as a function of the angle of incidence. Mathematically, this is equivalent to sending the neutron beam onto the film at at every energy but at a fixed angle of incidence. The film profile needs to be recovered from the measured reflectivity data. Unfortunately, the unique recovery is impossible, and many distinct unrelated profiles may correspond to the same reflectivity data.

In our DOE/EPSCoR sponsored research, we have developed an analytical method to uniquely recover the profile of a thin film from the measured reflectivity data. We have shown that by taking reflectivity measurements with two different substrates, one can uniquely determine the film profile. Previously, it was known that one could uniquely recover the profile by taking reflectivity measurements with three different substrates, and our findings indicate that the same goal can be accomplished by using fewer measurements.

At Mississippi State University we started an informal weekly seminar (called "the reflectometry meeting") at to attract various undergraduate and graduate students into the field. There were about 3 undergraduate students, 6 graduate students, and 2 faculty members attending these seminars.

The PI has collaborated with Dr. Norm Berk at National Institute of Standards and Technology (NIST) on various aspects of neutron reflectometry, from which various interesting problems of theoretical and practical importance have arisen. One of these problems is closely related to the important mathematical problem known as analytic extrapolation. Under appropriate conditions (known to hold in neutron reflectometry), the reflection data taken in a finite interval of neutron energies uniquely determines the data at all energies. Even though the uniqueness is assured mathematically, there are currently no available methods for analytic extrapolation. Currently, we are working on this problem as it arises in neutron reflectometry and looking for mathematical and numerical methods to extrapolate reflection data to higher and lower neutron energies. A solution to this problem is expected to have a big impact not only in neutron reflectometry, but in many areas of physics and engineering.

The PI has collaborated with Prof. Paul Sacks of Iowa State University, Prof. Daniil Sarkissian of Mississippi State University, and Prof. Levon Babadzanjanz of St. Petersburg State University, Russia on mathematical and numerical aspects of neutron reflectometry. These researchers jointly worked with the PI towards the preparation of numerical routines to extract the film profile from the reflection data.

We have prepared a Mathematica interface running Fortran 95 algorithms to produce reflection data from a given profile. These Fortran 95 algorithms have been prepared by updating and modifying Prof. Sacks' Fortran 77 routine and by updating Dr. Gian Felcher's (of Argonne National Laboratory) Fortran 77 routine. We are also preparing similar algorithms written in Mathematica so that they can be used without needing Fortran. We are also working towards preparing algorithms in Fortran 95 and in Mathematica to produce the film profile from the given sets of reflectivity data.

Publications acknowledging the DOE support

[1]. T. Aktosun, M. Klaus, and C. van der Mee, *Small-energy asymptotics of the scattering matrix for the matrix Schrödinger equation on the line,* Journal of Mathematical Physics **42** (2001) 4627-4657.

[2]. T. Aktosun and M. Klaus, *Inverse theory: problem on the line,* Chapter 2.2.4 in: Scattering (edited by E. R. Pike and P. C. Sabatier, Academic Press, London, 2001). pp. 770–785.

[3]. T. Aktosun and P. E. Sacks, *Potential splitting and numerical solution of the inverse scattering problem on the line,* Mathematical Methods in the Applied Sciences **25**

(2002) 347–355.

[4]. T. Aktosun and J. H. Rose, Wave focusing on the line, *Journal of Mathematical Physics* **43** (2002), 3717–3745.

[5]. T. Aktosun and R. Weder, Inverse scattering with partial information on the potential, *Journal of Mathematical Analysis and Applications* **270** (2002), 247–266.

[6]. T. Aktosun and V. G. Papanicolaou, Recovery of a potential from the ratio of reflection and transmission coefficients, *Journal of Mathematical Physics* **44** (2003), 4875–4883.

[7]. T. Aktosun, Construction of the half-line potential from the Jost function, *Inverse Problems* **20** (2004), 859–876.

[8]. T. Aktosun, Inverse scattering transform, KdV, and solitons, In: J. A. Ball, J. W. Helton, M. Klaus, and L. Rodman (eds.), *Current trends in operator theory and its applications,* Operator Theory: Advances and Applications, Vol. **149**, Birkhäuser, Basel, 2004, pp. 1–22.

[9]. T. Aktosun, V. G. Papanicolaou, and V. Zisis, Inverse scattering on the line for a generalized nonlinear Schrödinger equation, *Inverse Problems* **20** (2004), 1267–1280.

[10]. T. Aktosun, Inverse scattering on the line with incomplete scattering data, In: C. Conca, R. Manásevich, G. Uhlmann, and M. S. Vogelius (eds.), *Partial differential equations and inverse problems,* Contemporary Mathematics, Vol. **362**, American Mathematical Society, Providence, 2004, pp. 1–11.

[11]. T. Aktosun, Inverse scattering for vowel articulation with frequency-domain data, *Inverse Problems* **21** (2005), 899–914.

[12]. T. Aktosun, M. H. Borkowski, A. J. Cramer, and L. C. Pittman, Inverse scattering with rational scattering coefficients and wave propagation in nonhomogeneous media, In: R. Kaashoek, S. Seatzu, and C. van der Mee (eds.), *Current trends in operator theory and its applications,* Operator Theory: Advances and Applications, Vol. **160**, Birkhäuser, Basel, 2005, pp. 1–20.

[13]. T. Aktosun, Solitons and inverse scattering transform, In: D. P. Clemence and Guoqing Tang (eds.), *Mathematical studies in nonlinear wave propagation,* Contemporary

Mathematics, Vol. **379**, American Mathematical Society, Providence, 2005, pp. 47–62.

[14]. T. Aktosun and R. Weder, Inverse spectral-scattering problem with two sets of discrete spectra for the radial Schrödinger equation, Inverse Problems **22** (2006) , 89–114.